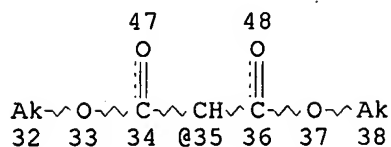
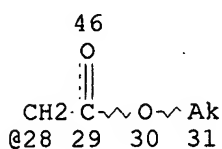
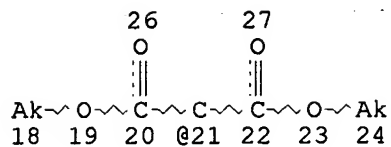
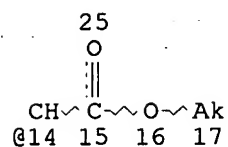
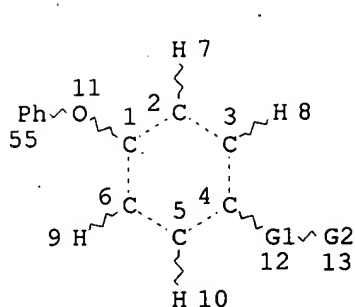


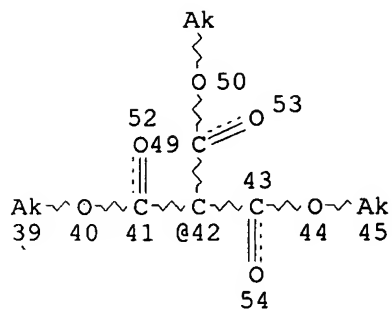
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L7

STR



51

Page 1-A



Page 2-A

VAR G1=CH2/14/21

VAR G2=CH3/28/35/42

NODE ATTRIBUTES:

CONNECT	IS	E1	RC	AT	17
CONNECT	IS	E1	RC	AT	18
CONNECT	IS	E1	RC	AT	24
CONNECT	IS	E1	RC	AT	31
CONNECT	IS	E1	RC	AT	32
CONNECT	IS	E1	RC	AT	38
CONNECT	IS	E1	RC	AT	39
CONNECT	IS	E1	RC	AT	45

CONNECT IS E1 RC AT 51  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE  
L9 8 SEA FILE=REGISTRY SSS FUL L7  
L10 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L9

=> d ibib abs hitstr ind l10 1-12

L10 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2001:546122 HCAPLUS  
DOCUMENT NUMBER: 135:257023  
TITLE: Palladium-catalyzed .alpha.-arylation of esters  
AUTHOR(S): Moradi, Wahed A.; Buchwald, Stephen L.  
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of  
Technology, Cambridge, MA, 02139, USA  
SOURCE: Journal of the American Chemical Society (2001),  
123(33), 7996-8002  
CODEN: JACSAT; ISSN: 0002-7863  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 135:257023

AB A new and simple one-pot procedure for the palladium-catalyzed intermol.  
.alpha.-arylation of esters is described. A no. of esters, e.g.  
MeCO<sub>2</sub>CMe<sub>3</sub>, can be functionalized with a wide range of aryl bromides, e.g.  
2-MeC<sub>6</sub>H<sub>4</sub>Br, using Pd(OAc)<sub>2</sub> or Pd<sub>2</sub>(dba)<sub>3</sub> and bulky electron-rich o-biphenyl  
phosphines. Under the reaction conditions, using LiHMDS as base,  
.alpha.-arylation proceeds at room temp. or at 80.degree.C with very good  
yields and high selectivities for monoarylation. Important nonsteroidal  
antiinflammatory drug derivs. such as (.+-.)-naproxen tert-Bu ester and  
(.+-.)-flurbiprofen tert-Bu ester can be prepd. in 79% and 86% yield,  
resp. The catalyst system based on the o-biphenyl contg. a dimethylamino  
group and di-tert-butylphosphine moiety is also active for the  
.alpha.-arylation of esters using aryl chlorides. Furthermore, using a  
bipnaphthyl di-tert-butylphosphine ligand, the .alpha.-arylation of  
trisubstituted ester enolates can be accomplished to provide compds. that  
have quaternary centers.

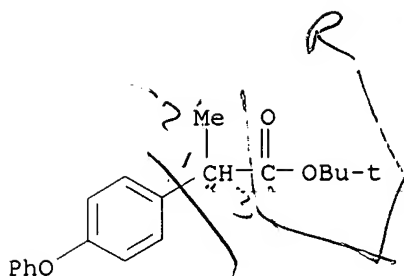
IT 362523-48-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(palladium-catalyzed .alpha.-arylation of esters with aryl halides  
using biphenyl/binaphthyl phosphine ligands)

RN 362523-48-6 HCAPLUS

CN Benzeneacetic acid, .alpha.-methyl-4-phenoxy-, 1,1-dimethylethyl ester  
(9CI) (CA INDEX NAME)

NAS



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 ST arylation ester palladium biphenyl binaphthyl ligand catalyst  
 IT Arylation  
 Arylation catalysts  
 (palladium-catalyzed .alpha.-arylation of esters with aryl halides  
 using biphenyl/binaphthyl phosphine ligands)  
 IT Aryl halides  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (palladium-catalyzed .alpha.-arylation of esters with aryl halides  
 using biphenyl/binaphthyl phosphine ligands)  
 IT 3375-31-3, palladium(II) acetate 51364-51-3, Pd2(dba)3 213697-53-1  
 224311-49-3 224311-52-8  
 RL: CAT (Catalyst use); USES (Uses)  
 (palladium-catalyzed .alpha.-arylation of esters with aryl halides  
 using biphenyl/binaphthyl phosphine ligands)  
 IT 92-66-0, 1-Bromo-4-phenylbenzene 95-46-5, 2-Bromotoluene 101-55-3,  
 1-Bromo-4-phenoxybenzene 101-97-3, Ethyl 2-phenylacetate 103-64-0,  
 1-Bromo-2-phenylethene 106-38-7, 4-Bromotoluene 106-43-4,  
 4-Chlorotoluene 108-37-2, 1-Bromo-3-chlorobenzene 401-78-5,  
 1-Bromo-3-(trifluoromethyl)benzene 460-00-4, 1-Bromo-4-fluorobenzene  
 540-88-5, tert-Butyl acetate 576-22-7, 1-Bromo-2,6-dimethylbenzene  
 580-13-2, 2-Bromonaphthalene 586-77-6, 1-Bromo-4-(dimethylamino)benzene  
 623-12-1, 1-Chloro-4-methoxybenzene 2039-88-5, 1-Bromo-2-vinylbenzene  
 2308-38-5, tert-Butyl butanoate 5111-65-9, 2-Bromo-6-methoxynaphthalene  
 5892-99-9 7005-72-3, 1-Chloro-4-phenoxybenzene 7073-94-1,  
 1-Bromo-2-(isopropyl)benzene 7452-79-1, Ethyl 2-methylbutanoate  
 20487-40-5, tert-Butyl propanoate 23786-14-3 41604-19-7,  
 1,1'-Biphenyl, 4-bromo-2-fluoro 59247-47-1, tert-Butyl 4-bromobenzoate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (palladium-catalyzed .alpha.-arylation of esters with aryl halides  
 using biphenyl/binaphthyl phosphine ligands)  
 IT 5359-57-9P 5589-35-5P 33155-60-1P 62381-17-3P 63860-06-0P  
 68825-45-6P 93579-03-4P 124853-54-9P 138623-00-4P 138623-03-7P  
 362523-40-8P 362523-41-9P 362523-42-0P 362523-43-1P 362523-44-2P  
 362523-45-3P 362523-46-4P 362523-47-5P **362523-48-6P**  
 362523-49-7P 362523-50-0P 362523-51-1P 362523-52-2P 362523-53-3P  
 362523-54-4P 362523-55-5P 362523-56-6P 362523-57-7P 362523-58-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (palladium-catalyzed .alpha.-arylation of esters with aryl halides  
 using biphenyl/binaphthyl phosphine ligands)  
 REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2001:279024 HCAPLUS  
 DOCUMENT NUMBER: 135:92596  
 TITLE: Novel 5,5-disubstituted pyrimidine-2,4,6-triones as  
 selective MMP inhibitors  
 AUTHOR(S): Foley, L. H.; Palermo, R.; Dunten, P.; Wang, P.

CORPORATE SOURCE: Roche Research Center, Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(8), 969-972

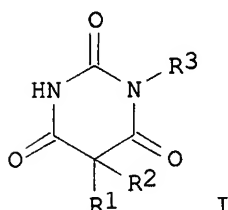
PUBLISHER: CODEN: BMCLE8; ISSN: 0960-894X

DOCUMENT TYPE: Elsevier Science Ltd.

LANGUAGE: Journal

OTHER SOURCE(S): English

GI CASREACT 135:92596



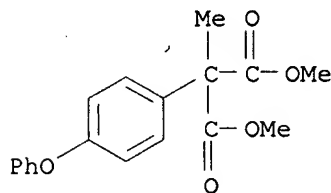
AB The 5,5-disubstituted pyrimidine-2,4,6-triones I (R1 = H, Me, Et hexyl, HOCH2CH2, PhCH2OCH2; R2 = Ph, 4-PhC6H4, 4-PhOC6H4, 4-octyl-OC6H4; R3 = H, Me) were prepd. and shown to be a novel and non-toxic class of matrix metalloproteinase (MMP) inhibitors showing selectivity for the gelatinases A and B, collagenase-3, and human neutrophil collagenase. The selectivities shown for MMPs-2, -8, -9, and -13 make I very attractive antitumor agents.

IT 349148-14-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

RN 349148-14-7 HCAPLUS

CN Propanedioic acid, methyl(4-phenoxyphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)



CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

ST pyrimidine trione prepn gelatinase inhibitor; matrix metalloprotein inhibitor pyrimidine trione

IT Antitumor agents  
(prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

IT 288102-94-3P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent).  
 (prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

IT 76-94-8P 67051-21-2P 94209-48-0P 219311-20-3P 288102-95-4P  
 288102-96-5P 288102-97-6P 288102-99-8P 349148-09-0P 349148-10-3P  
 349148-11-4P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

IT 146480-35-5, Gelatinase A 146480-36-6, Gelatinase B  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

IT 21490-51-7 65749-05-5 288103-00-4 288103-01-5 288103-02-6  
 288103-04-8 349148-12-5 349148-13-6 **349148-14-7**  
 349148-15-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of disubstituted pyrimidine triones as selective matrix metalloprotein (MMP) inhibitors)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:44662 HCAPLUS

DOCUMENT NUMBER: 126:59751

TITLE: Preparation of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors

INVENTOR(S): Baker, William R.; Rosenberg, Saul H.; Fung, K. L. Anthony; Rockway, Todd W.; Fakhoury, Stephen A.; Garvey, David S.; Donner, B. Gregory; O'Connor, Stephen J.; Prasad, Rajnandan N.; Shen, Wang; Stout, David M.; Sullivan, Gerard M.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 241 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9634851	A1	19961107	WO 1996-US6193	19960502
W: AU, CA, JP, KR, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5783593	A	19980721	US 1996-633262	19960429
AU 9656731	A1	19961121	AU 1996-56731	19960502
PRIORITY APPLN. INFO.:			US 1995-429095	19950503
			US 1996-633262	19960429
			US 1993-147708	19931104

US 1994-289711

19940909

US 1994-322783

19941018

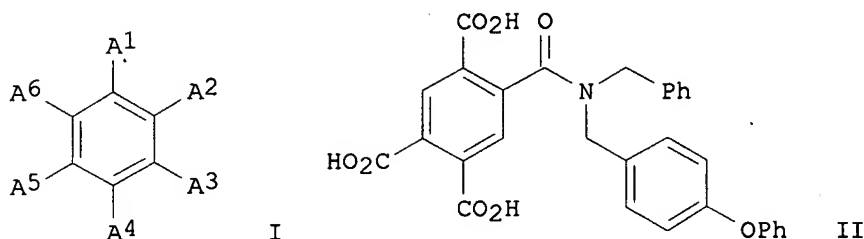
WO 1996-US6193

19960502

OTHER SOURCE(S):

MARPAT 126:59751

GI



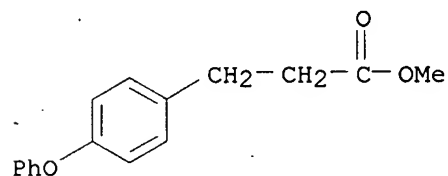
AB Title compds. [e.g., I; A1 = ZCONR1R2; A2, A4, and A5 or A2 and A4 or A3 and A4 = (protected) CO<sub>2</sub>H and the other An = H; R1 = (chloro)benzyl, (CH<sub>2</sub>)<sub>2</sub>-4Ph, CH<sub>2</sub>C<sub>6</sub>H<sub>4</sub>(OPh)-4; R2 = (CH<sub>2</sub>)<sub>1</sub>-2C<sub>6</sub>H<sub>4</sub>(OPh)-4; Z = bond, NR, O; R = H, (cyclo)alkyl, aralkyl, cycloalkylalkyl] were prep'd. Thus, 4-(PhO)C<sub>6</sub>H<sub>4</sub>CHO was reductively aminated by H<sub>2</sub>CH<sub>2</sub>Ph and the product amidated by 1,2,4,5-benzenetetracarboxylic dianhydride to give title comp'd. II. Data for in vitro inhibition of protein farnesyltransferase by selected I were given.

IT 185051-02-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

RN 185051-02-9 HCAPLUS

CN Benzenepropanoic acid, 4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07C233-73

ICS C07C233-65; C07C235-38; C07D257-04; C07C275-42; C07C335-22;  
C07C233-12; C07D333-20

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1

ST carboxybenzamide squalene synthetase protein farnesyltransferase inhibitor

IT Artery, disease

(coronary, restenosis, prevention; prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT Ras proteins

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(farnesylation; prepn. of di- and tricarboxybenzamides and analogs as

squalene synthetase and protein farnesyltransferase inhibitors)

IT Antitumor agents  
(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT 185047-82-9P 185047-83-0P 185047-84-1P 185047-85-2P 185047-86-3P  
 185047-87-4P 185047-88-5P 185047-89-6P 185047-90-9P 185047-91-0P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT 131384-38-8, Protein farnesyltransferase  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
 (prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT 170433-63-3P, 1,2-Benzenedicarboxylic acid, 4-hydroxymethyl-, dimethyl

ester

RL: BYP (Byproduct); PREP (Preparation)

(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

IT 61-54-1, 3-(2-Aminoethyl)indole 65-49-6, 4-Aminosalicylic acid  
 67-36-7, 4-Phenoxybenzaldehyde 85-44-9, 1,3-Isobenzofurandione 89-32-7  
 89-51-0, Homophthalic acid 89-57-6, 5-Aminosalicylic acid 89-93-0,  
 2-Methylbenzylamine 93-09-4, 2-Naphthoic acid 93-55-0, Propiophenone  
 95-48-7, reactions 95-65-8, 3,4-Dimethylphenol 96-32-2, Methyl  
 bromoacetate 99-63-8, 1,3-Benzenedicarbonyl dichloride 100-20-9,  
 1,4-Benzenedicarbonyl dichloride 100-39-0, Benzyl bromide 100-46-9,  
 Benzylamine, reactions 100-51-6, Benzyl alcohol, reactions 100-52-7,  
 Benzaldehyde, reactions 100-81-2, 3-Methylbenzylamine 101-53-1,  
 4-Hydroxydiphenylmethane 103-49-1, Dibenzylamine 103-63-9, Phenethyl  
 bromide 106-44-5, 4-Methylphenol, reactions 106-48-9, 4-Chlorophenol  
 108-39-4, 3-Methylphenol, reactions 118-31-0, 1-Naphthylmethylamine  
 138-25-0 150-76-5, 4-Methoxyphenol 459-57-4, 4-Fluorobenzaldehyde  
 527-60-6, 2,4,6-Trimethylphenol 552-30-7 556-56-9, Allyl iodide  
 569-51-7, 1,2,3-Benzenetricarboxylic acid 610-22-0, Dimethyl  
 4-nitrophthalate 699-98-9, 2,3-Pyridinedicarboxylic anhydride  
 703-59-3, Homophthalic anhydride 1204-28-0, 4-Chlorocarbonylphthalic  
 anhydride 1758-46-9, 2-Phenoxyethylamine 1955-46-0, 3-Nitroisophthalic  
 acid monomethyl ester 2038-57-5, Benzenepropanamine 2045-79-6,  
 2-Methoxyphenethylamine 2217-40-5, 1-Amino-1,2,3,4-Tetrahydronaphthalene  
 2270-20-4, 5-Phenylpentanoic acid 2393-23-9, 4-Methoxybenzylamine  
 2420-87-3, [5,5'-Biisobenzofuran]-1,1',3,3'-tetrone 2421-28-5  
 2426-87-1, 4-Benzyloxy-3-methoxybenzaldehyde 2672-58-4,  
 1,3,5-Benzenetricarboxylic acid, trimethyl ester 2687-43-6,  
 O-Benzylhydroxylamine hydrochloride 2740-83-2, 3-  
 Trifluoromethylbenzylamine 2835-06-5 2975-41-9, 2-Aminoindane  
 3048-01-9, 2-Trifluoromethylbenzylamine 3082-77-7, L-Methionine ethyl  
 ester 3113-72-2, 5-Methyl-2-nitrobenzoic acid 3132-99-8,  
 3-Bromobenzaldehyde 3218-02-8, Cyclohexanemethanamine 3218-36-8,  
 4-Phenylbenzaldehyde 3669-48-5 3711-01-1, 2,3,6,7-  
 Naphthalenetetracarboxylic dianhydride 3731-51-9, 2-Pyridylmethylamine  
 3731-52-0, 3-Pyridylmethylamine 3731-53-1, 4-Pyridylmethylamine  
 3939-09-1, 2,4-Difluorobenzonitrile 4360-51-4, 1-Amino-3-phenyl-2-  
 propene 4393-09-3, 2,3-Dimethoxybenzylamine 4397-53-9,  
 4-Benzyloxybenzaldehyde 4442-59-5, 1,4-Benzodioxan-2-methylamine  
 4821-94-7, 4,5-Dimethoxyphthalic anhydride 5326-47-6,  
 2-Amino-5-iodobenzoic acid 5372-81-6, Dimethyl aminoterephthalate  
 5470-84-8, 4-Benzyloxybutyraldehyde 5736-88-9, 4-Butoxybenzaldehyde  
 5870-38-2, Diethyl 2,5-dihydroxyterephthalate 5927-18-4,  
 Trimethylphosphonoacetate 6050-13-1, Diphenic anhydride 6287-38-3,  
 3,4-Dichlorobenzaldehyde 6328-74-1, 4-Phenoxyphenylacetic acid  
 6850-57-3, 2-Methoxybenzylamine 6921-34-2, Benzylmagnesium chloride  
 7355-22-8, 5-Bromo-2,4-dihydroxybenzoic acid 7409-30-5,  
 4-Nitrobenzylamine 7617-76-7, 3-Phenoxypropylamine 7745-93-9,  
 2-Bromo-4-nitrotoluene 13214-66-9, 4-Phenylbutylamine 17532-66-0,  
 1,2-Benzenediacetic acid, diethyl ester 18655-51-1, 3-(2-  
 Methoxyphenyl)propylamine 19014-14-3 19434-34-5, 2-Phenoxybenzaldehyde  
 20116-65-8, Dimethyl 4-methylphthalate 20781-22-0 22117-85-7  
 22440-62-6 22479-95-4, Dimethyl 4-hydroxyphthalate 24541-01-3,  
 4-Chromanone oxime 24850-33-7, Allyltributyltin 26759-46-6  
 27757-85-3, 2-Thiophenemethanamine 28994-41-4, 2-Hydroxydiphenylmethane  
 34698-41-4, 1-Aminoindane 37806-29-4, 2-Ethoxybenzylamine 37806-49-8,  
 Benzenemethanamine, 2-(3-methylbutoxy)- 37806-66-9 39515-51-0,



3-Phenoxybenzaldehyde 39590-27-7, Benzenethanamine, 2-ethoxy-  
 40663-68-1, 4-Allyloxybenzaldehyde 42116-44-9, N-tert-  
 Butoxycarbonylbenzenemethanamine 58332-00-6 60728-41-8 69770-20-3,  
 3-(4-Chlorophenoxy)benzaldehyde 69770-23-6, 3-(4-tert-  
 Butylphenoxy)benzaldehyde 72235-53-1, 3,4-Difluorobenzylamine  
 79124-75-7, 3-(4-Methylphenoxy)benzaldehyde 79124-76-8,  
 3-(3,4-Dichlorophenoxy)benzaldehyde 88088-95-3, Tris(1-  
 benzotriazolyl)methane 107624-14-6, Benzenemethanamine, 2-phenoxy-  
 165534-79-2, Dimethyl iodoterephthalate 169943-62-8 169943-64-0  
 171350-07-5 171350-08-6 184229-19-4, 4-Phenoxy-3-chlorobenzaldehyde  
 185051-61-0 185051-62-1 185051-63-2 185051-64-3,  
 N-Benzyl-2-fluorenylmethylamine

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of di- and tricarboxybenzamides and analogs as squalene  
 synthetase and protein farnesyltransferase inhibitors)

IT 2215-84-1P 3786-39-8P 3898-66-6P 4315-09-7P, 4-Nitrobenzene-1,3-  
 dicarboxylic acid 16426-64-5P 19241-40-8P 20116-67-0P,  
 1,2-Benzenedicarboxylic acid, 4-bromomethyl-, dimethyl ester 29710-58-5P  
 38588-64-6P, 1,3,5-Benzenetricarboxylic acid, dimethyl ester  
 39585-32-5P, Benzenecetic acid, 2-carboxy-5-nitro- 40172-06-3P,  
 N-(3,4-Dichlorobenzyl)ethanolamine 46253-86-5P 51832-31-6P, Dimethyl  
 4-aminophthalate 52446-51-2P, 2-(4-Phenoxyphenyl)ethanol 53981-38-7P;  
 4-Aminochroman 60313-18-0P 63746-12-3P, Dimethyl 4-aminoisophthalate  
 64481-29-4P 67402-72-6P 68872-14-0P 69048-70-0P, Dimethyl  
 4-nitroisophthalate 74733-34-9P 76784-89-9P, Benzenecetic acid,  
 5-amino-2-(methoxycarbonyl)-, methyl ester 79807-86-6P 91345-28-7P  
 91963-85-8P 100959-22-6P, Methyl 2-bromo-4-nitrobenzoate 110786-89-5P,  
 1,2-Benzenedicarboxylic acid, 4-mercapto-, dimethyl ester 129951-06-0P,  
 Benzenebutanamine, N-phenylmethyl- 136534-67-3P, Benzenepentanamine,  
 N-phenylmethyl- 138408-68-1P, Methyl 4-hydroxy-2-methoxy-5-vinylbenzoate  
 144146-84-9P, N-Benzyl-5-phenylpentanamide 147810-06-8P 169943-97-9P,  
 N-Benzyl-N-(4-phenoxybenzyl)amine 170433-65-5P, Dimethyl  
 4-(carboxymethyl)phthalate 179056-63-4P 179098-29-4P 184033-42-9P,  
 4-tert-Butoxycarbonylamino-2-hydroxybenzoic acid 184228-76-0P  
 184228-77-1P 184228-78-2P 184228-79-3P 185050-26-4P 185050-27-5P  
 185050-28-6P 185050-29-7P 185050-30-0P 185050-31-1P 185050-32-2P,  
 2-Cyano-5-iodobenzoic acid 185050-33-3P 185050-34-4P 185050-35-5P  
 185050-36-6P 185050-37-7P 185050-38-8P 185050-39-9P 185050-40-2P  
 185050-41-3P 185050-42-4P 185050-43-5P 185050-44-6P 185050-45-7P  
 185050-46-8P 185050-47-9P 185050-48-0P 185050-49-1P 185050-50-4P  
 185050-51-5P 185050-52-6P 185050-53-7P 185050-54-8P 185050-55-9P  
 185050-56-0P 185050-57-1P 185050-58-2P 185050-59-3P 185050-60-6P  
 185050-61-7P 185050-62-8P 185050-63-9P 185050-64-0P 185050-65-1P  
 185050-66-2P 185050-67-3P 185050-68-4P 185050-69-5P 185050-70-8P  
 185050-71-9P 185050-72-0P 185050-73-1P 185050-74-2P 185050-75-3P  
 185050-76-4P 185050-77-5P, Methyl 5-bromo-4-hydroxy-2-methoxybenzoate  
 185050-78-6P 185050-79-7P, Methyl 2-methoxy-4,5-divinylbenzoate  
 185050-80-0P, 2-Methoxy-4,5-divinylbenzoic acid 185050-81-1P  
 185050-82-2P 185050-83-3P 185050-84-4P 185050-85-5P 185050-86-6P  
 185050-87-7P 185050-88-8P 185050-89-9P 185050-90-2P 185050-91-3P  
 185050-92-4P 185050-93-5P 185050-94-6P, Methyl 4-tert-  
 Butoxycarbonylamino-2-hydroxybenzoate 185050-95-7P 185050-96-8P  
 185050-97-9P 185050-98-0P 185050-99-1P 185051-00-7P 185051-01-8P  
**185051-02-9P** 185051-03-0P 185051-04-1P 185051-05-2P  
 185051-06-3P 185051-07-4P 185051-08-5P 185051-09-6P 185051-10-9P  
 185051-11-0P 185051-12-1P 185051-13-2P 185051-14-3P 185051-15-4P  
 185051-16-5P 185051-17-6P 185051-18-7P 185051-19-8P 185051-20-1P

185051-21-2P	185051-22-3P	185051-23-4P	185051-24-5P	185051-25-6P
185051-26-7P	185051-27-8P	185051-28-9P	185051-29-0P	185051-30-3P
185051-31-4P	185051-32-5P	185051-33-6P	185051-34-7P	185051-35-8P
185051-36-9P	185051-37-0P	185051-38-1P	185051-39-2P	185051-40-5P
185051-41-6P	185051-42-7P	185051-43-8P	185051-44-9P	185051-45-0P
185051-46-1P	185051-47-2P	185051-48-3P	185051-49-4P	185051-50-7P
185051-51-8P	185051-52-9P	185051-53-0P	185051-54-1P	185051-55-2P
185051-56-3P	185051-57-4P	185051-58-5P	185051-59-6P	185051-60-9P
185051-67-6P	185230-57-3P			

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of di- and tricarboxybenzamides and analogs as squalene synthetase and protein farnesyltransferase inhibitors)

L10 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:442116 HCAPLUS

DOCUMENT NUMBER: 121:42116

TITLE: Study on the source of nonvolatile mutagenic organics in the water of East Lake and the tap water from it

AUTHOR(S): Tian, Shizhong; Huang, Zhidan; Deng, Nansheng; Zhang, Jiayao; Zhao, Pihong; Xiao, Mei; Liu, Dazhi; Zhizhong, Jing; Meilan, Wang; Xizhao, Yuan

CORPORATE SOURCE: Dep. Environ. Sci., Wuhan Univ., Wuhan, 430072, Peop. Rep. China

SOURCE: Zhongguo Huanjing Kexue (1993), 13(2), 100-5

CODEN: ZHKKEI; ISSN: 1000-6923

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB A total of 102 org. pollutants (alkylbenzenes, polycyclic arom. hydrocarbons, phthalic esters, etc.) in East Lake and the tap water from it were identified by gas chromatog.-mass spectrometry. Ames test results showed that they have mutagenicity to TA98, and are direct mutagens. Model test of chlorination of humic acid or fulvic acid showed that humics of low concn. in water do not form nonvolatile mutagenic orgs. and nonvolatile mutagenic orgs. in the tap water from East Lake.

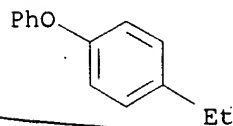
IT 36207-23-5

RL: BIOL (Biological study)

(lake water and potable water pollution by, Salmonella typhimurium toxicity in relation to, of East Lake, China)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



CC 61-2 (Water)

Section cross-reference(s): 4, 10

ST org water pollution East Lake China; Salmonella typhimurium toxicity org lake pollution; Ames test toxicity org water pollution

IT Water pollution

(by org. compds., of lake water and potable water, Salmonella typhimurium toxicity in relation to, of East Lake, China)

IT Organic compounds, biological studies

RL: BIOL (Biological study)

(lake water and potable water pollution by, *Salmonella typhimurium* toxicity in relation to, of East Lake, China)

IT Toxicity

(of org. compds. in polluted lake water and potable water, to *Salmonella typhimurium* strain TA-98, Ames test detn. of, of East Lake, China)

IT *Salmonella typhimurium*

(strain TA-98, polluted lake and potable water toxicity to, Ames test for, of East Lake, China)

IT 57-10-3, Hexadecanoic acid, biological studies 64-19-7, Acetic acid, biological studies 67-66-3, Trichloromethane, biological studies 71-43-2, Benzene, biological studies 75-27-4, Bromodichloromethane 75-65-0, Tert-Butanol, biological studies 84-66-2, Diethyl phthalate 84-69-5, Diisobutyl phthalate 84-74-2, Dibutyl phthalate 86-73-7, Fluorene 91-20-3, Naphthalene, biological studies 95-16-9, Benzothiazole 95-50-1, o-Dichlorobenzene 100-41-4, Ethylbenzene, biological studies 100-42-5, biological studies 100-52-7, Benzaldehyde, biological studies 106-46-7, p-Dichlorobenzene 108-88-3, Toluene, biological studies 108-90-7, Chlorobenzene, biological studies 110-54-3, Hexane, biological studies 110-82-7, Cyclohexane, biological studies 110-93-0, 6-Methyl-5-heptene-2-one 111-27-3, Hexanol, biological studies 111-65-9, Octane, biological studies 111-84-2, Nonane 112-30-1, Decanol 112-95-8, Eicosane 117-81-7, Dioctyl phthalate 120-12-7, Anthracene, biological studies 124-48-1, Dibromochloromethane 128-37-0, 2,6-Ditert-butyl-4-methylphenol, biological studies 128-39-2, 2,6-Di-tert-butylphenol 131-11-3 140-29-4, Benzylcyanide 206-44-0, Fluoranthene 486-25-9, 9H-Fluoren-9-one 489-84-9 535-77-3, 1-Methyl-3-isopropylbenzene 541-73-1, m-Dichlorobenzene 544-63-8, Tetradecanoic acid, biological studies 593-45-3, Octadecane 629-78-7, Heptadecane 629-92-5, Nonadecane 629-94-7, Heneicosane 629-97-0, Docosane 646-31-1, Tetracosane 678-26-2, Perfluoropentane 719-22-2 763-93-9, 3-Hexen-2-one 814-78-8 934-34-9, Benzothiazolone 937-30-4 1138-52-9, 3,5-Di-tert-butylphenol 1331-43-7, Diethylcyclohexane 1569-50-2, 3-Pentene-2-ol 1689-78-7, 2-tert-Butylthiophene 2142-64-5 2219-82-1, 2-tert-Butyl-6-methylphenol 2245-30-9 2444-28-2, 2,6-Di-tert-butyl-1,4-benzenediol 4130-42-1, 2,6-Di-tert-butyl-4-ethylphenol 4281-40-7 4562-27-0, 4-1H)-Pyrimidinone 4675-87-0 4920-99-4, 1-Ethyl-3-isopropylbenzene 7507-89-3 11071-47-9, Isooctene 12002-48-1, Trichlorobenzene 15356-74-8 18794-47-3 19377-95-8 24270-68-6, 1,1,2,3-Tetrafluoropropane 25377-83-7, Octene 25378-22-7, Dodecene 25495-91-4, Bromohexane 27138-19-8, Ethylnaphthalene 27195-67-1, Dimethylcyclohexane 27400-77-7, Nonadecene 27400-79-9, Heneicosene 28351-09-9, Dimethylbenzaldehyde 28804-88-8, Dimethylnaphthalene 29253-36-9, Isopropyl-naphthalene 29512-02-5, 1-Methoxy-1-butene 29730-67-4, Docosene 34314-83-5, 4-Methyl-2,3-dihydrofuran 34464-40-9, Isononane 34970-00-8, Iodobromochloromethane 36207-23-5 53951-50-1, Ethylbenzaldehyde 58501-92-1 61923-54-4, 2-Penten-2-ol 62808-70-2 103502-85-8 156000-89-4 156057-47-5

RL: BIOL (Biological study)

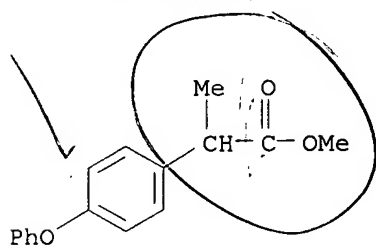
(lake water and potable water pollution by, *Salmonella typhimurium* toxicity in relation to, of East Lake, China)

L10 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 1990:206735 HCAPLUS

DOCUMENT NUMBER: 112:206735  
 TITLE: Preparation of .alpha.-arylacetic acid derivatives by electrochemical oxidation  
 INVENTOR(S): Shono, Tatsuya; Matsumura, Isahiro  
 PATENT ASSIGNEE(S): Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01222078	A2	19890905	JP 1988-50233	19880302

PRIORITY APPLN. INFO.: JP 1988-50233 19880302  
 OTHER SOURCE(S): MARPAT 112:206735  
 AB A method for prepg. ACRR1COOR2 (A = aryl, (condensed) heterocyclic group; R,R1 = H, alkyl, alicyclic group, unsatd. hydrocarbon group, aryl, aralkyl; R2 = H or lower alkyl) involves electrochem. oxidn. of ACOCHRR1 in the presence of I (or its compd.) and an acetalization agent.  
 IT 126934-95-0P  
 RL: PREP (Preparation)  
 (prepn. of, electrochem., by oxidn. of ketone derivs.)  
 RN 126934-95-0 HCAPLUS  
 CN Benzeneacetic acid, .alpha.-methyl-4-phenoxy-, methyl ester (9CI) (CA INDEX NAME)



IC ICM G25B003-02  
 CC 72-9 (Electrochemistry)  
 ST arylacetic acid prepn electrochem oxidn ketone  
 IT Oxidation, electrochemical  
 (of ketones, in prepn. of arylacetic acid derivs.)  
 IT 74-88-4, uses and miscellaneous 149-73-5 7553-56-2, Iodine, uses and miscellaneous  
 RL: PROC (Process)  
 (electrochem. oxidn. of ketones in presence of, for prepn. of arylacetic acid derivs.)  
 IT 75-30-9 75-47-8 591-50-4 3240-34-4 7553-56-2, Iodine, uses and miscellaneous 7681-11-0, Potassium iodide (KI), uses and miscellaneous 7758-05-6 10034-85-2, Hydriodic acid 12027-06-4, Ammonium iodide ((NH4)I) 16029-98-4  
 RL: PROC (Process)  
 (electrochem. oxidn. of ketones in presence of, in prepn. of arylacetic acid derivs.)  
 IT 93-55-0 98-86-2, reactions 495-40-9 582-62-7 611-70-1 712-50-5 889-26-9 1515-95-3 2700-47-2 6315-96-4 10342-83-3 52129-98-3 59771-24-3 66952-37-2 80336-83-0 114012-26-9 120703-45-9

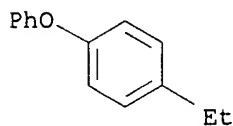
126916-32-3 126934-92-7 126934-93-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (electrochem. oxidn. of, in prepn. of arylacetic acid derivs.)  
 IT 101-41-7P 2294-71-5P 17380-78-8P 30012-51-2P 31508-44-8P  
 50415-73-1P 52263-88-4P 57421-64-4P 57625-74-8P 59235-36-8P  
 61566-34-5P 66202-87-7P 72615-27-1P 73913-50-5P 83636-46-8P  
 103392-12-7P 120703-46-0P 125670-62-4P 126934-94-9P  
**126934-95-0P** 126934-96-1P  
 RL: PREP (Preparation)  
 (prepn. of, electrochem., by oxidn. of ketone derivs.)

L10 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1990:97962 HCAPLUS  
 DOCUMENT NUMBER: 112:97962  
 TITLE: Reactivity of ring-substituted ethylbenzenes in  
 reactions with cumylperoxy radicals  
 AUTHOR(S): Efimova, I. V.; Matvienko, A. G.; Opeida, I. A.  
 CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., Donetsk, USSR  
 SOURCE: Zhurnal Organicheskoi Khimii (1989), 25(4), 801-4  
 CODEN: ZORKAE; ISSN: 0514-7492  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB The reaction const.  $\rho$  [detd. from  $\sigma$  + substituent consts. in  
 p-RC<sub>6</sub>H<sub>4</sub>Et (I)] for the H-abstraction reaction with PhCMe<sub>2</sub>OO $\cdot$  was more  
 statistically reliable than  $\rho$ , reflecting the significant contribution  
 of polar conjugation of R with the reaction center in transition-state  
 stabilization. The abs. magnitude of  $\rho$ , on the basis of current and  
 literature evaluations, decreased in the series RC<sub>6</sub>H<sub>4</sub>Me > I > RC<sub>6</sub>H<sub>4</sub>CHMe<sub>2</sub>,  
 reflecting the Hammond reactivity-selectivity principle.

IT **36207-23-5**  
 RL: PRP (Properties)  
 (abstraction reaction of hydrogen of, with cumylperoxy radical,  
 kinetics of)

RN 36207-23-5 HCAPLUS  
 CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



CC 22-13 (Physical Organic Chemistry)  
 ST abstraction hydrogen ethylbenzene deriv kinetics; substituent effect  
 hydrogen abstraction ethylbenzene; reaction const hydrogen abstraction  
 ethylbenzene; benzene alkyl reactivity selectivity  
 IT Reaction constant  
 (for abstraction reaction of hydrogen from ethylbenzene derivs. with  
 cumylperoxy radical)  
 IT Kinetics of abstraction reaction  
 (of hydrogen, from ethylbenzene derivs. with cumylperoxy radical)  
 IT Substituent effect  
 (on abstraction reaction of hydrogen from ethylbenzene derivs. with  
 cumylperoxy radical)  
 IT 141-93-5, m-Diethylbenzene 937-30-4, p-Acetyethylbenzene 1515-95-3,  
 p-Methoxyethylbenzene 1585-07-5, p-Bromoethylbenzene **36207-23-5**

RL: PRP (Properties)  
 (abstraction reaction of hydrogen of, with cumylperoxy radical,  
 kinetics of)

IT 7175-54-4, Cumylperoxy radical

RL: PRP (Properties)  
 (abstraction reaction of hydrogen of, with ethylbenzene derivs.,  
 kinetics of)

L10 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1989:594298 HCAPLUS

DOCUMENT NUMBER: 111:194298

TITLE: Preparation of substituted phenylpropionaldehydes as  
 drug intermediates

INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao

PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.  
 CODEN: JKXXAF

DOCUMENT TYPE: Patent

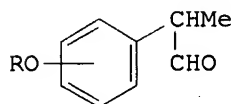
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290837	A2	19881128	JP 1987-125683	19870525
PRIORITY APPLN. INFO.:			JP 1987-125683	19870525
OTHER SOURCE(S):		MARPAT 111:194298		

GI



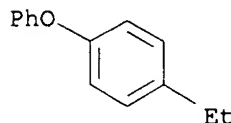
AB The title compds. I (R = Ph, Me), useful as drug intermediates, were  
 prepd. Dehydrogenation of 3-phenoxyphenylethane, followed by  
 hydroformylation of the product in the presence of (Ph<sub>3</sub>P)3Rh(CO)H under H  
 and CO, gave 2-(3-phenoxyphenyl)propionaldehyde with 91% selectivity and  
 99.1% conversion of 3-phenoxyphenylethylene.

IT 36207-23-5, 4-Phenoxyphenylethane

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydrogenation of)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



IC ICM C07C047-277  
 ICS C07C045-50

CC 25-15 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
Section cross-reference(s): 1

ST phenylpropionaldehyde prepn drug intermediate; fenoprofen intermediate  
phenylpropionaldehyde prepn; hydroformylation phenylethylene

IT Hydroformylation  
(of phenylethylenes)

IT 17185-29-4, Hydridocarbonyltris(triphenylphosphine)rhodium  
RL: CAT (Catalyst use); USES (Uses)  
(catalyst, for hydroformylation of phenylethylenes)

IT 1515-95-3 10568-38-4, 3-Methoxyphenylethane **36207-23-5**,  
4-Phenoxyphenylethane 78427-95-9, 3-Phenoxyphenylethane  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(dehydrogenation of)

IT 20401-88-1P 40138-66-7P 54954-44-8P 122801-83-6P  
RL: SPN (Synthetic preparation); FORM (Formation, nonpreparative); PREP  
(Preparation)  
(formation of, in prepn. of drug intermediate)

IT 630-08-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydroformylation, of phenylethylenes)

IT 29679-58-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(intermediates for, prepn. of phenylpropionaldehydes as)

IT 626-20-0P 637-69-4P, 4-Methoxyphenylethylene 4973-29-9P,  
4-Phenoxyphenylethylene 63444-54-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and hydroformylation of)

IT 5405-83-4P 59452-86-7P 59908-87-1P 80793-26-6P 123490-60-8P  
123490-61-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as drug intermediate)

L10 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1989:231286 HCAPLUS

DOCUMENT NUMBER: 110:231286

TITLE: Process for the preparation of 2-(substituted  
phenyl)propionates as pharmaceuticals or their  
intermediates

INVENTOR(S): Takahashi, Eiji; Ozaki, Kazuo; Yamada, Takao

PATENT ASSIGNEE(S): Maruzen Petrochemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

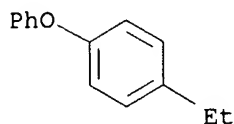
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63290842	A2	19881128	JP 1987-125684	19870525
PRIORITY APPLN. INFO.:			JP 1987-125684	19870525
OTHER SOURCE(S):			MARPAT 110:231286	

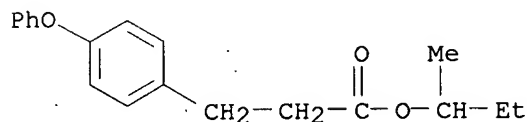
AB Title compds. R1OC6H4CHMeCO2R2 (R1 = Ph, Me; R2 = H, alkyl), e.g.  
phenopropylene, are prepd. by dehydrogenation of R1OC6H4Et in the presence  
of a dehydrogenation catalyst at 400-700.degree. and carbonylation of the  
resultant R1OC6H4CH:CH2 in H2O or an alc. in the presence of a Pd

catalyst. 3-PhOC6H4Et and H2O at 0.5 h<sup>-1</sup> LHSV were charged in a reactor contg. tin oxide at 580.degree., to give 3-PhOC6H4CH:CH2 in 61.3% yield, and the product was autoclaved with Me2CHOH, PdCl2(PPh3)2, PPh3, and 35% HCl at 110.degree. and 120 kg/cm2 CO to give total 99.8% yield of 3-PhOC6H4CHMeCO2CHMe2 and 3-PhOC6H4(CH2)2CO2CHMe2 (93.2% and 6.4% selectivity, resp.).

IT **36207-23-5**, 4-Phenoxyphenylethane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydrogenation of, styrene deriv. from)  
 RN 36207-23-5 HCAPLUS  
 CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



IT **120824-60-4P**, sec-Butyl 3-(4-phenoxyphenyl)propionate  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 RN 120824-60-4 HCAPLUS  
 CN Benzenepropanoic acid, 4-phenoxy-, 1-methylpropyl ester (9CI) (CA INDEX NAME)



IC ICM C07C059-64  
 ICS B01J031-22; C07C051-14; C07C067-38; C07C069-734  
 CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 1  
 ST phenylpropionate prepn pharmaceutical intermediate  
 IT Pharmaceuticals  
 (intermediates for, phenylpropionates as)  
 IT Alkoxy carbonylation  
 (of styrene derivs., phenylpropionates from)  
 IT 1515-95-3, 4-Methoxyphenylethane 10568-38-4, 3-Methoxyphenylethane  
**36207-23-5**, 4-Phenoxyphenylethane 78427-95-9,  
 3-Phenoxyphenylethane  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (dehydrogenation of, styrene deriv. from)  
 IT 4973-29-9P, 4-Phenoxyphenylethylene 10568-38-4P, 3-Methoxyphenylethane  
 78427-95-9P, 3-Phenoxyphenylethane  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and alkoxy carbonylation of)  
 IT 637-69-4P, 4-Methoxyphenylethylene  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and alkoxy carbonylation of)  
 IT 113777-15-4P, Isopropyl 3-(3-methoxyphenyl)propionate 120824-59-1P,



Isopropyl 3-(3-phenoxyphenyl)propionate 120824-60-4P, sec-Butyl  
3-(4-phenoxyphenyl)propionate 120824-61-5P, sec-Butyl  
3-(4-methoxyphenyl)propionate

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

IT 120824-55-7P, Isopropyl 2-(3-phenoxyphenyl)propionate 120824-56-8P,  
sec-Butyl 2-(3-phenoxyphenyl)propionate 120824-57-9P, sec-Butyl  
2-(4-methoxyphenyl)propionate 120824-58-0P, Isopropyl  
2-(3-methoxyphenyl)propionate

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for drugs)

L10 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1984:551531 HCAPLUS

DOCUMENT NUMBER: 101:151531

TITLE: Thallium in organic synthesis. 62. A convenient  
synthesis of .alpha.-arylsuccinic acids

AUTHOR(S): Taylor, Edward C.; Conley, Richard A.; Katz, Alan H.;  
McKillop, Alexander

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA

SOURCE: Journal of Organic Chemistry (1984), 49(20), 3840-1

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 101:151531

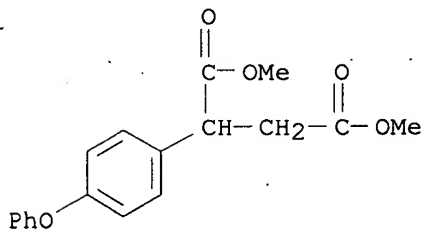
AB .alpha.-Arylsuccinic acids are readily prepd. by oxidative rearrangement  
of .beta.-aroylpropionic acids (from arenes and succinic anhydride) with  
Tl(NO3)3- -HC(OMe)3. Application of the same reaction to  
.beta.-benzoylbutyric acid, .beta.-benzoylvaleric acid,  
1,2-dibenzoylthane and 1,4-dibenzoylbutane gives di-Me  
.alpha.-phenylglutarate, di-Me .alpha.-phenyladipate, di-Me  
.alpha.,.alpha.'-diphenylsuccinate, and di-Me .alpha.,.alpha.'-  
diphenyladipate, resp. Oxidative rearrangement of unsym.  
1,2-diaroylthanes gives unsym. di-Me .alpha.,.alpha.'-diarylsuccinates.

IT 91266-19-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by oxidative rearrangement of benzoylalkanoic acid with  
thallium trinitrate and tri-Me orthoformate)

RN 91266-19-2 HCAPLUS

CN Butanedioic acid, (4-phenoxyphenyl)-, dimethyl ester (9CI) (CA INDEX  
NAME)



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST benzoylalkanoic acid oxidative rearrangement; benzoylalkane di oxidative  
rearrangement; alkanolic acid benzoyl oxidative rearrangement; alkane  
dibenzoyl oxidative rearrangement; oxidative rearrangement dibenzoylalkane

benzoylalkanoic acid; thallium nitrate oxidative rearrangement

IT Oxidation  
(rearrangement and, of benzoylalkanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)

IT Rearrangement  
(oxidative, of benzoylalkanoic acids and dibenzoylalkanes with thallium trinitrate and tri-Me orthoformate, diesters by)

IT 5447-74-5 25333-24-8 39560-31-1 57498-54-1 67173-95-9 91266-23-8  
RL: PROC (Process)  
(conversion of, to enol ether)

IT 366-77-8 495-71-6 2051-95-8 3153-44-4 3375-38-0 4144-62-1  
4619-20-9 36330-86-6 51908-41-9 89229-73-2 91266-20-5 91266-21-6  
91266-22-7 91266-24-9 91266-25-0 91266-26-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidative rearrangement of, with thallium trinitrate and tri-Me orthoformate)

IT 1496-23-7P 10436-86-9P 15463-92-0P 22248-26-6P 36265-44-8P  
81631-72-3P **91266-19-2P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by oxidative rearrangement of benzoylalkanoic acid with thallium trinitrate and tri-Me orthoformate)

IT 7300-04-1P 19020-59-8P 91280-66-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by oxidative rearrangement of dibenzoylalkane with thallium nitrate and tri-Me orthoformate)

IT 149-73-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(thallium trinitrate and, oxidative rearrangement of benzoylalkanoic acids and dibenzoylalkanes by)

IT 13746-98-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(tri-Me orthoformate and, oxidative rearrangement of benzoylalkanoic acids and dibenzoylalkanes by)

L10 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:467848 HCAPLUS

DOCUMENT NUMBER: 87:67848

TITLE: .alpha.-Aryl-substituted propionic acids

INVENTOR(S): Takeda, Makoto; Uchide, Masayuka; Iwane, Hiroshi

PATENT ASSIGNEE(S): Mitsubishi Petrochemical Co., Ltd., Japan

SOURCE: Ger. Offen., 43 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

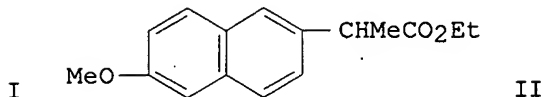
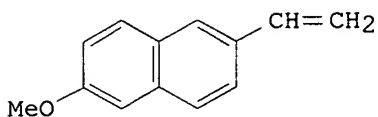
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2646792	A1	19770428	DE 1976-2646792	19761016
DE 2646792	C2	19850509		
JP 52051338	A2	19770425	JP 1975-127787	19751023
JP 59035899	B4	19840831		
JP 60045171	B4	19851008	JP 1976-91523	19760731
GB 1565235	A	19800416	GB 1976-43221	19761018
FR 2328689	A1	19770520	FR 1976-32143	19761025
FR 2328689	B1	19830121		

US 4329507 A 19820511 US 1980-111978 19800114  
 PRIORITY APPLN. INFO.: JP 1975-127787 19751023  
 JP 1976-91523 19760731  
 US 1976-734592 19761021  
 US 1978-909643 19780525

GI



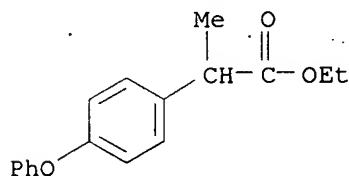
AB Alkoxyacylation by alcs. and CO and carboxylation by H<sub>2</sub>O and CO of vinylarenes were catalyzed by Pd complexes. Thus, I in EtOH contg. (Ph<sub>3</sub>P)<sub>2</sub>PdCl<sub>2</sub>, BF<sub>3</sub>·Et<sub>2</sub>O, and Ph<sub>2</sub>NNO was autoclaved with CO to give 69% II.

IT 61001-75-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and hydrolysis of)

RN 61001-75-0 HCAPLUS

CN Benzeneacetic acid, .alpha.-methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



IC C07C069-76

CC 23-16 (Aliphatic Compounds)

Section cross-reference(s): 25, 26

ST alkoxyacylation vinylarene catalyst; carboxylation vinylarene catalyst; propionic acid aryl

IT Alkoxyacylation catalysts  
 (palladium complexes, for vinylarenes)

IT 5338-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Grignard reaction of)

IT 391-08-2 716-89-2 3139-85-3 4973-29-9 10473-10-6 30215-52-2

54314-33-9 63444-51-9 63444-52-0 63444-53-1 63444-54-2

63444-55-3 63444-56-4 63444-57-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (alkoxyacylation of)

IT 109-63-7 603-35-0, uses and miscellaneous 7647-10-1 13965-03-2  
 14977-08-3

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for alkoxyacylation of vinylarenes)

IT 62049-65-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(dehydrochlorination of)

IT 5002-42-6 42771-85-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydride redn. of)

IT 40150-92-3P 56430-69-4P 63444-59-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and dehydration of)

IT 56430-44-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and dehydrohalogenation of)

IT 37961-57-2P 41283-72-1P **61001-75-0P** 61566-34-5P  
63444-58-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and hydrolysis of)

IT 3585-53-3P 5005-84-5P 6908-47-0P 15687-27-1P 17692-38-5P  
22410-97-5P 23981-80-8P 29679-58-1P 36141-62-5P 36950-96-6P  
41604-03-9P 51106-57-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

L10 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:592403 HCAPLUS

DOCUMENT NUMBER: 85:192403

TITLE: Phenoxyphenylbutyric acid derivatives

INVENTOR(S): Gante, Joachim; Kurmeier, Hans A.; Schacht, Erich;

Mehrhof, Werner; Wild, Albrecht

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 51 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

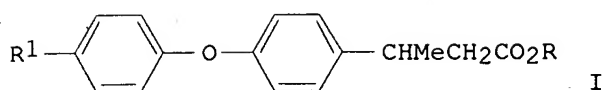
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2509891	A1	19760923	DE 1975-2509891	19750307
SE 7602744	A	19760908	SE 1976-2744	19760227
AU 7611555	A1	19770908	AU 1976-11555	19760302
AU 497104	B2	19781130		
BE 839211	A2	19760906	BE 1976-7000789	19760304
FR 2302731	A1	19761001	FR 1976-6130	19760304
DK 7600979	A	19760908	DK 1976-979	19760305
NL 7602341	A	19760909	NL 1976-2341	19760305
ZA 7601340	A	19770223	ZA 1976-1340	19760305
ES 445793	A1	19770901	ES 1976-445793	19760305
GB 1494462	A	19771207	GB 1976-8980	19760305
AT 7601624	A	19790515	AT 1976-1624	19760305
JP 51125348	A2	19761101	JP 1976-25990	19760308
			DE 1975-2509891	19750307

PRIORITY APPLN. INFO.:

GI



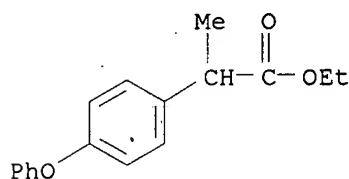
AB The title compounds (I; R = H, Me, Et, Pr, Bu, tert-Bu, Et2NCH2CH2, Me2NCH2CH2; R1 = H, Br, Cl, F), useful as analgesics and antipyretics, are prepd. by a variety of std. procedures. Thus, redn. and hydrolysis of 4-(4-ClC6H4O)C6H4CMe(OH)CH2CO2Et with 67% aq. HI in AcOH 1 hr at 150.degree. gives I (R = H, R1 = Cl).

IT 61001-75-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of)

RN 61001-75-0 HCAPLUS

CN Benzeneacetic acid, .alpha.-methyl-4-phenoxy-, ethyl ester (9CI) (CA INDEX NAME)



IC C07C069-76

CC 25-18 (Noncondensed Aromatic Compounds)

ST phenoxyphenylbutyrate analgesic antipyretic; butyrate halophenoxyphenyl analgesic antipyretic

IT Analgesics

Antipyretics

((halophenoxy)phenyl]butyrate acid derivs.)

IT 55102-99-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with K 3-iodobutyrate)

IT 61001-87-4 61001-88-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with carbon dioxide)

IT 78-09-1 124-38-9, reactions 541-41-3 61001-86-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Grignard reaction with halophenyl ethers)

IT 61001-75-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(chlorination of)

IT 61001-98-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(deamination and fluoroamination of)

IT 61001-97-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
(deamination of)

IT 61001-90-9 61001-91-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(decarboxylation of)

IT 60467-98-3 61001-74-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrogenation and hydrolysis of)  
IT 61001-76-1 61024-36-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrogenation of)  
IT 61001-89-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis and decarboxylation of)  
IT 58727-42-7 58727-45-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis and redn. of)  
IT 61001-78-3 61001-79-4 61001-80-7 61001-81-8 61001-82-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(hydrolysis of)  
IT 58727-63-2 61001-94-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidn. of)  
IT 61001-57-8P 61001-61-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and esterification of)  
IT 61001-58-9P 61001-64-7P 61001-65-8P 61001-66-9P 61001-67-0P  
61001-71-6P 61001-72-7P 61001-73-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(prepn. and hydrolysis of)  
IT 61001-59-0P 61001-60-3P 61001-63-6P 61001-68-1P 61001-70-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)  
IT 1099-45-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with 4-(1-bromoethyl)-4'-fluorodiphenyl ether)  
IT 61024-35-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with carbon monoxide)  
IT 1951-12-8 7425-49-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with chlorophenyl phenyl ether)  
IT 61001-95-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with diethylamine)  
IT 352-34-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with disodium 3-(4-hydroxyphenyl)butyrate)  
IT 61001-77-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with ethyl [triphenylphosphoranylidene)acetate)  
IT 61001-83-0 61001-84-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with ethyl bromobutyrate)  
IT 61024-34-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with fluoroiodobenzene)  
IT 61001-93-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with formic acid and with nickel carbonyl)  
IT 7005-72-3  
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction with halobutyrate)

IT 13463-39-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with halophenyl ethers)

IT 61001-92-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with nickel carbonyl)

IT 100-35-6 107-99-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with sodium [(chlorophenoxy)phenyl]butyrate)

IT 61001-96-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with sodium fluorophenolate)

IT 61001-85-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with tert-butyl alc. and propanol)

IT 371-35-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction with sodium (iodophenyl)butyrate)

IT 64-18-6, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(with 4-chlorophenyl 4-(2-propenyl)phenyl ether)

IT 630-08-0, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(with [(chlorophenoxy)phenyl]propanol)

IT 109-89-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(with chloroethyl [(chlorophenoxy)phenyl]butyrate)

L10 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1972:144751 HCAPLUS

DOCUMENT NUMBER: 76:144751

TITLE: Effect of introducing ethyl radical to benzene derivatives on their odorant properties

AUTHOR(S): Wizner, Iwonna

CORPORATE SOURCE: Inst. Chem. Przem., Warsaw, Pol.

SOURCE: Tluszcz, Srodki Piorace, Kosmetyki (1971), 15(5), 20-30

CODEN: TSPKBZ; ISSN: 0372-1795

DOCUMENT TYPE: Journal

LANGUAGE: Polish

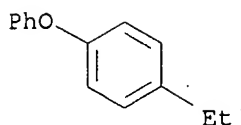
AB The effects of Et groups on odorant properties was studied in large no. of esters, alcs., aldehydes, and ketones, as well as in p-ethyl diphenylmethane (I) and p-ethyl diphenyl ether. The most interesting scent was found in p-ethylacetophenone, I, Me p-ethylbenzoate, and p-ethylphenyl-.beta.-butyl alc. Many of the compds. synthesized are not found in literature.

IT 36207-23-5

RL: PRP (Properties)  
(odors of)

RN 36207-23-5 HCAPLUS

CN Benzene, 1-ethyl-4-phenoxy- (9CI) (CA INDEX NAME)



- CC 62 (Essential Oils and Cosmetics)
- ST ethyl groups odorant; ester odorant ethyl effect; alc odorant ethyl effect; aldehyde odorant ethyl effect; ketone odorant ethyl effect
- IT Molecular structure-property relationship  
(benzene ethyl derivs., odors)
- IT Alcohols, properties  
Aldehydes, properties  
Esters, properties  
Ketones, properties  
RL: PRP (Properties)  
(odors of, ethyl radicals in relation to)
- IT Odor and Odorous substances  
(of benzene ethyl derivs.)
- IT 768-59-2 4748-78-1 14062-20-5 22545-13-7 36207-03-1 36207-04-2  
36207-05-3 36207-06-4 36207-07-5 36207-08-6 36207-09-7  
36207-10-0 36207-13-3 36207-14-4 36207-15-5 36207-16-6  
36207-18-8 36207-19-9 36305-78-9  
RL: PRP (Properties)  
(odor of)
- IT 620-85-9 937-30-4 7364-20-7 **36207-23-5**  
RL: PRP (Properties)  
(odors of)
- IT 36207-25-7P  
RL: PREP (Preparation)  
(prepn. of)